

Claims

I claim:

- 1 1. A method of measuring the molecular mass of a compound Y of unknown
2 molecular mass by mass spectrometry, comprising
3 providing a sample of compound Y,
4 providing samples of at least two different compounds each of Formula (I), R-X in
5 which R is a trityl group and X is cleavable to form a charged species for mass spectrometry,
6 and recording the molecular mass of compound Y and the at least two compounds
7 of Formula (I) in a mass spectrometer.
- 1 2. The method, according to claim 1, in which R is R¹R²R³ C- wherein R¹, R² and
2 R³ are the same or different and each is a monocyclic or fused ring aromatic group that is
3 substituted or unsubstituted.
- 1 3. The method, according to claim 2, in which at least one of R¹, R² and R³ carries
2 a substituent selected from the group consisting of substituted or unsubstituted C₁-C₂₀ alkoxy
3 and hydrocarbyl.
- 1 4. The method, according to claim 3, in which the alkoxy or hydrocarbyl is
2 substituted by a substituent selected from the group consisting of carboxylic acid, sulphonic
3 acid, nitro, cyano, hydroxyl, thiol, primary, secondary or tertiary amino, primary or secondary
4 amido, anhydride, carbonyl halide and active ester.
- 1 5. The method, according to any of claim 2, in which each of R¹, R² and R³ is aryl.
- 1 6. The method, according to claim 5, wherein said aryl is phenyl.

1 7. The method, according to claim 1, in which the trityl group R has at least two
2 amide substituents.

1 8. The method, according to claim 7, wherein said trityl group R has at least four
2 amide substituents.

1 9. The method, according claim 2, in which R¹, R² and R³ together carry at least two
2 amide groups and/or at least two reactive groups for coupling.

1 10. The method, according to claim 9, wherein said groups are N-hydroxy
2 succinimide ester groups.

1 11. The method, according to claim 1, in which X is halide or tosylate.

1 12. The method, according to claim 1, comprising providing at least five compounds
2 of Formula (I) and recording their molecular masses in a mass spectrometer.

1 13. The method, according claim 1, in which the group X is photocleavable to form
2 a charged species for mass spectrometry.

1 14. The method, according to claim 1, additionally comprising estimating the
2 molecular mass of unknown compound Y as M_y and providing at least one compound of
3 Formula (I) which has known molecular mass M₁ below M_y and at least one different
4 compound of Formula (I) which has molecular mass M₂ above M_y.

1 15. The method, according to claim 14, wherein the difference between M_y and each
2 of M₁ and M₂ is not more than ±50%.

1 16. The method, according to claim 1, additionally comprising providing a sample
2 of at least one further compound Z of unknown molecular mass and measuring the molecular
3 mass of compound Z.

1 ✓ 17. Use of a compound of Formula (I) R-X in which R is a trityl group and X is
2 cleavable to form a charged species for mass spectrometry as a calibration compound for
3 mass spectrometry.

1 ✓ 18. A kit for the production of calibration compounds for mass spectrometry
2 comprising:

3 (a) at least one base reactant of Formula (I) R-X where R is a trityl group and X is
4 cleavable to form a charged species for mass spectrometry; and

5 (b) at least two different amine compounds which are of different molecular masses
6 and which are each capable of reacting with the base reactant;

7 wherein the base reactant (a) is packaged separately from amine compounds (b).

1 19. The kit, according to claim 18, additionally comprising instructions to select at
2 least two desired molecular masses M_1 and M_2 for the calibration compounds and to choose
3 one or more amines for reaction with the base reactant so as to obtain compounds of the
4 desired predetermined molecular masses M_1 and M_2 , and instructions to use the compounds
5 in mass spectrometry.

1 ✓ 20. A set of calibration compounds for mass spectrometry comprising at least two
2 separately packaged mixtures (a) and (b), wherein

3 mixture (a) comprises at least two different compounds each of formula (I) R-X and
4 having different molecular masses, and

5 mixture (b) comprises at least two further compounds of formula (I) R-X having
6 different molecular masses and wherein R is a trityl group and X is cleavable to form a
7 charged species for mass spectrometry.

1 21. The set, according to claim 20, in which the lowest molecular mass in mixture
2 (a) is lower than the lowest molecular mass in mixture (b) and the highest molecular mass
3 in mixture (a) is lower than the highest molecular mass in mixture (b).

1 22. The set, according to claim 20, in which each of mixtures (a) and (b) contains at
2 least five different compounds of different molecular masses.

1 23. The set, according to claim 22, in which each of mixtures (a) and (b) contains at
2 least 10 different compounds of different molecular masses.

1 24. The set, according to claim 20, comprising at least three separately packaged
2 mixtures of compounds.

1 25. The set, according to claim 24, comprising at least five separately packaged
2 mixtures of compounds.

1 26. A kit for the production of a set of calibration compounds comprising a first
2 package comprising a base reactant of Formula (I) R-X, in which R is a trityl group and X
3 is cleavable to form a charged species for mass spectrometry, and at least two separate
4 second packages (a) and (b), each containing a mixture of at least two amine compounds
5 which have different molecular masses and which are capable of reacting with the base
6 reactant.

1 27. The kit, according to claim 26, in which the lowest molecular mass in mixture
2 (a) is lower than the lowest molecular mass in mixture (b) and the highest molecular mass
3 in mixture (a) is lower than the highest molecular mass in mixture (b).

1 28. The kit, according to claim 26, in which each of mixtures (a) and (b) contain at
2 least five different amine compounds of different molecular masses.

1 29. The kit, according to claim 28, wherein each of mixtures (a) and (b) contain at
2 least ten different amine compounds of molecular masses.

1 30. The kit, according to claim 26, comprising at least three mixtures of amine
2 compounds.

1 31. The kit, according to claim 30, comprising at least five mixtures of amine
2 compounds.

1 32. A method of measuring the molecular mass of a compound Y of unknown
2 molecular mass comprising
3 estimating the expected molecular mass of compound Y, selecting at least one
4 calibration compound of Formula (I) R-X having molecular weight close to the expected
5 molecular weight of the compound Y, in which R is a trityl group and X is cleavable to form
6 a charged species for mass spectrometry
7 and subjecting both compounds to mass spectrometry simultaneously.

1 33. The method, according to claim 32, in which the calibration compound R-X is
2 provided by selecting a base reactant R-X and selecting an amine reactant of appropriate
3 molecular mass and reacting the amine reactant and the base reactant.

1 34. A mixture of at least two compounds of Formula (I) R-X in which R is a trityl
2 group and X is a group cleavable to give a charged species for analysis by mass spectrometry.

1 35. The mixture, according to claim 34, comprising at least five different compounds
2 of Formula (I).

1 36. The mixture, according to claim 35, comprising at least ten different compounds
2 of Formula (I).

1 37. A method of mass spectrometry comprising subjecting simultaneously to mass
2 spectrometry at least two different compounds of Formula (I) R-X in which R is a trityl
3 group and X is cleavable to give a charged species for analysis by mass spectrometry.